Pentanedioic acid, hexafluoro-376-73-8 | DTXSID8059926

Model Performance

Mode	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 8.09e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.50e-01

Confidence level: 3.67e-01

Nearest Neighbors from the Training Set

Image not found

Kepone

Measured: 2.34e-04 Predicted: 1.30e-07

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Ethyl acetate

Measured: 1.50e-03 Predicted: 89.2

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Acrylic acid

Measured: 2.00e-02 Predicted: 1.46

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Dimethoxymethane Measured: 1.91e-07 Predicted: 170

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Ethanediamide Measured: 4.64e-07 Predicted: 7.36e-08